Response of Graphs to Competing Constraints

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Abstract: We discuss recent proofs of both differentiable and singular responses of dense graphs as contraints on edge and triangle densities are varied. Proving differentiability requires control over typical (exponentially most) graphs with given sharp values of those two densities. Based on arxiv:2110.14052 (Joe Neeman, CR and Lorenzo Sadun).

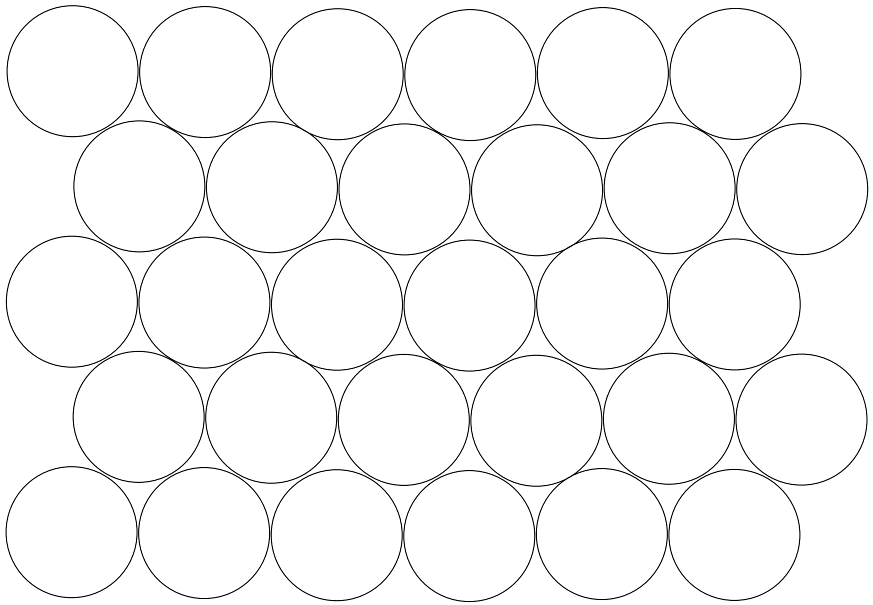
This talk is on the pure mathematics of large, dense graphs subjected to ‘competing constraints’. I emphasize the notion of competing constraints, and more specifically the *consequences in finite graphs* of such competition between constraints (‘tension’).

To give some perspective I begin with a quick review of competing constraints in two other combinatorial settings:

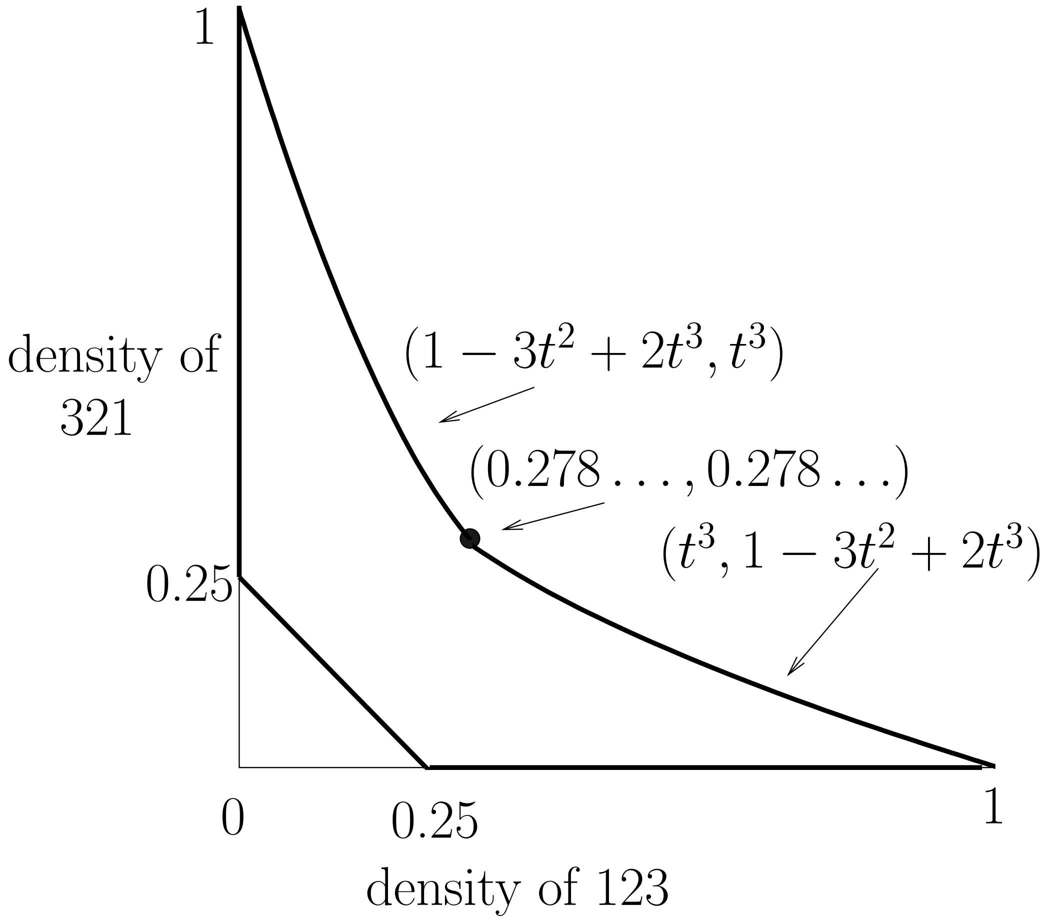
1) densest packing of unit spheres (covering fraction *vs.* no overlap)

2) permutations with extreme densities of patterns 123 and 321

1) The tension in packing problems is easily seen when trying to maximize covering fraction. For unit disks in the plane, the optimal configuration is unique: each disk surrounded by six others.



2) Among permutations the possible joint densities of the patterns 123 and 321 are shown in the following figure; certain portions of the edges exhibit the competition. Note the kink at (0.278, 0.278).



In both sphere packing and constrained permutations there is real interest in the 'states' (configurations/permutations) which achieve *extreme* constraints. Competition is seen there but is better explored in *nonextremely* constrained states, analyzing the effect of the competition on 'typical' states with such given constraints.

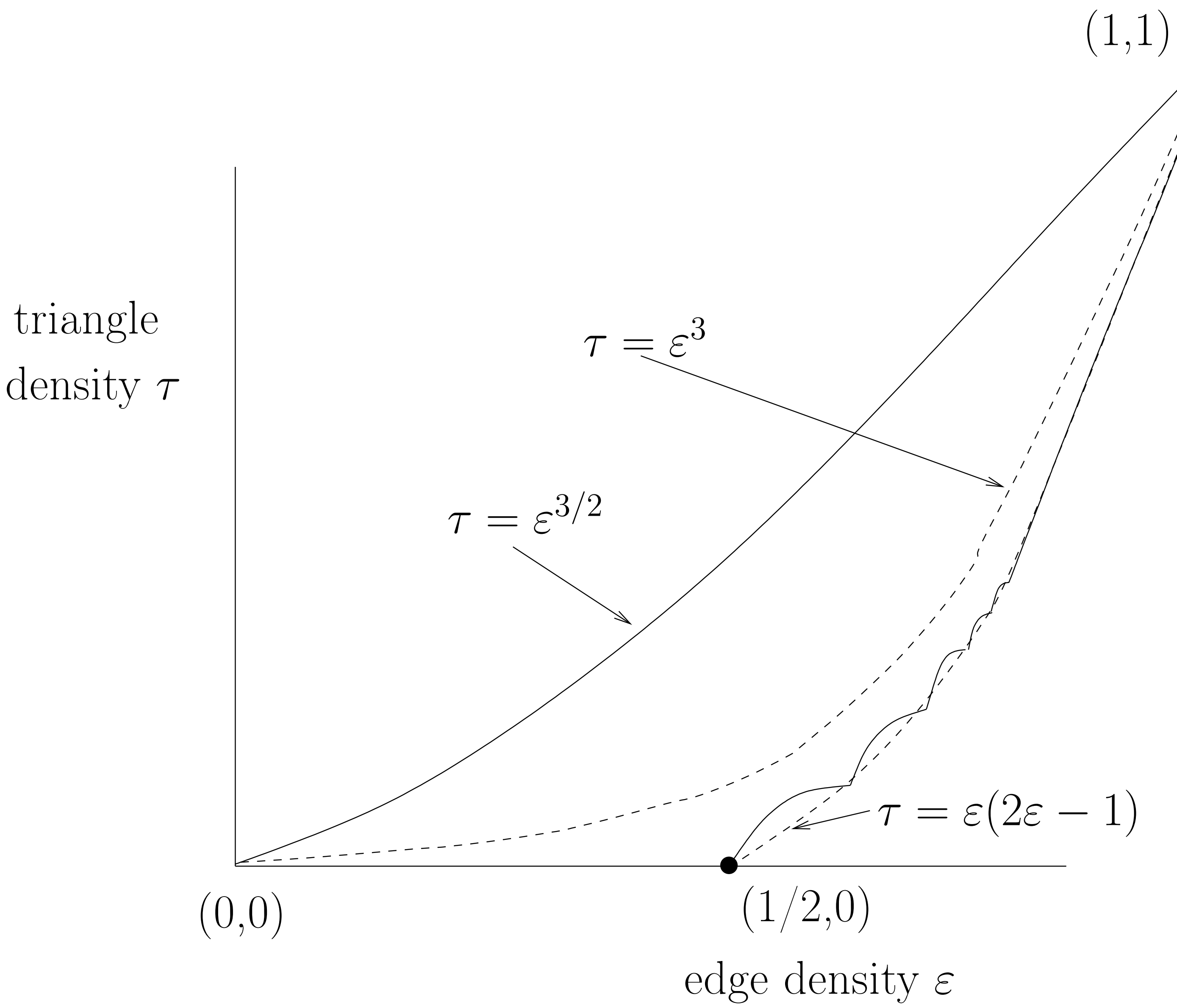
For example in dimension 2 one expects from simulations (1950's) that typical disk packings with high density remain ordered like the optimum as the covering fraction is decreased from the optimum of $\pi/\sqrt{12} \approx 0.91$ down to about 0.71 where the typical state changes sharply to become disordered – though this cannot be proven.

Also, the permutation kink might be expected to have effects in the interior, which in this case has been proven in Section 10 of:

R. Kenyon, D. Kráľ, CR and P. Winkler, Permutations with fixed pattern densities, Random Structures Algorithms 56(2020) 220-250.

Now on to constrained *graphs*, which is the best developed of these three 'competing constraints' combinatorial areas. More specifically we consider dense graphs at large but finite (fixed) n, with constraints on **edge** and **triangle** density.

This example from extremal graph theory is old. I start with its status in 2012 (Pikhurko/Razborov):


(1,1)
triangle
density τ
$\tau = \varepsilon^3$
$\tau = \varepsilon^{3/2}$
$\tau = \varepsilon(2\varepsilon - 1)$
(0,0)
(1/2,0)
edge density ε

Our new results concern *nonextreme* constraints, as in sphere packing and permutations above. The project began with:

C. Radin and L. Sadun, Phase transitions in a complex network, J. Phys. A: Math. Theor. 46(2013) 305002

And followed closely after:

Chatterjee/Varadhan (2010) LDP for $G(n,p)$, some ERGMs

Chatterjee/Diaconis (2011) more on ERGMs, esp edge/triangle

Pikhurko/Razborov (2012) extreme edge/triangle constraints

With (ε, τ) in the interior of the Razborov triangle, new thread began with the study of $Z_n(\varepsilon, \tau, \delta)$, the cardinality of the set of graphs on n nodes with edge density in the interval $(\varepsilon - \delta, \varepsilon + \delta)$ and triangle density in the interval $(\tau - \delta, \tau + \delta)$.

We first proved that the limits exist:

$$\lim_{\delta \to 0} \lim_{n \to \infty} (1/n^2) \ln[Z_n(\varepsilon, \tau, \delta)] = s_{\varepsilon,\tau}$$

and that this 'Boltzmann entropy' can be represented as follows:

Variational principle for Boltzmann entropy

$$s_{\varepsilon,\tau} = \max_{t_\varepsilon(q)=\varepsilon, t_\tau(q)=\tau} S(q),$$

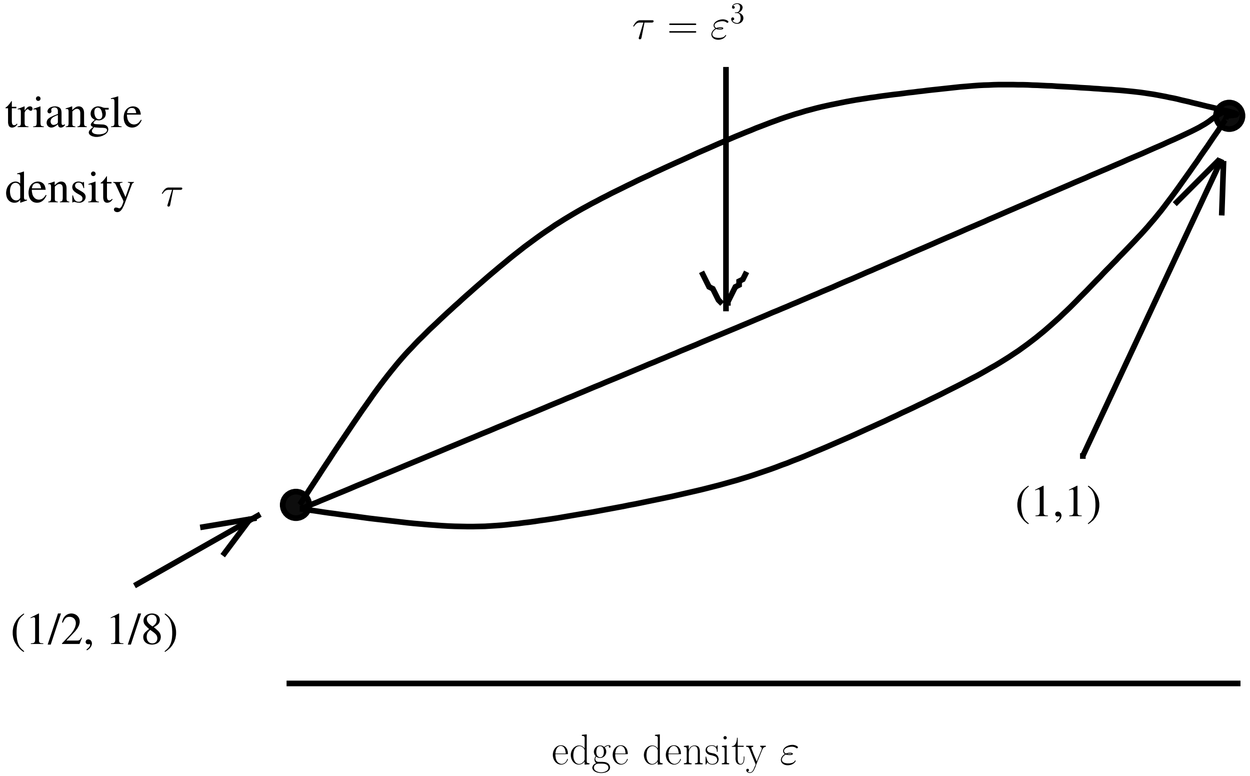
where $S(q)$ is the 'Shannon entropy' of graphon q:

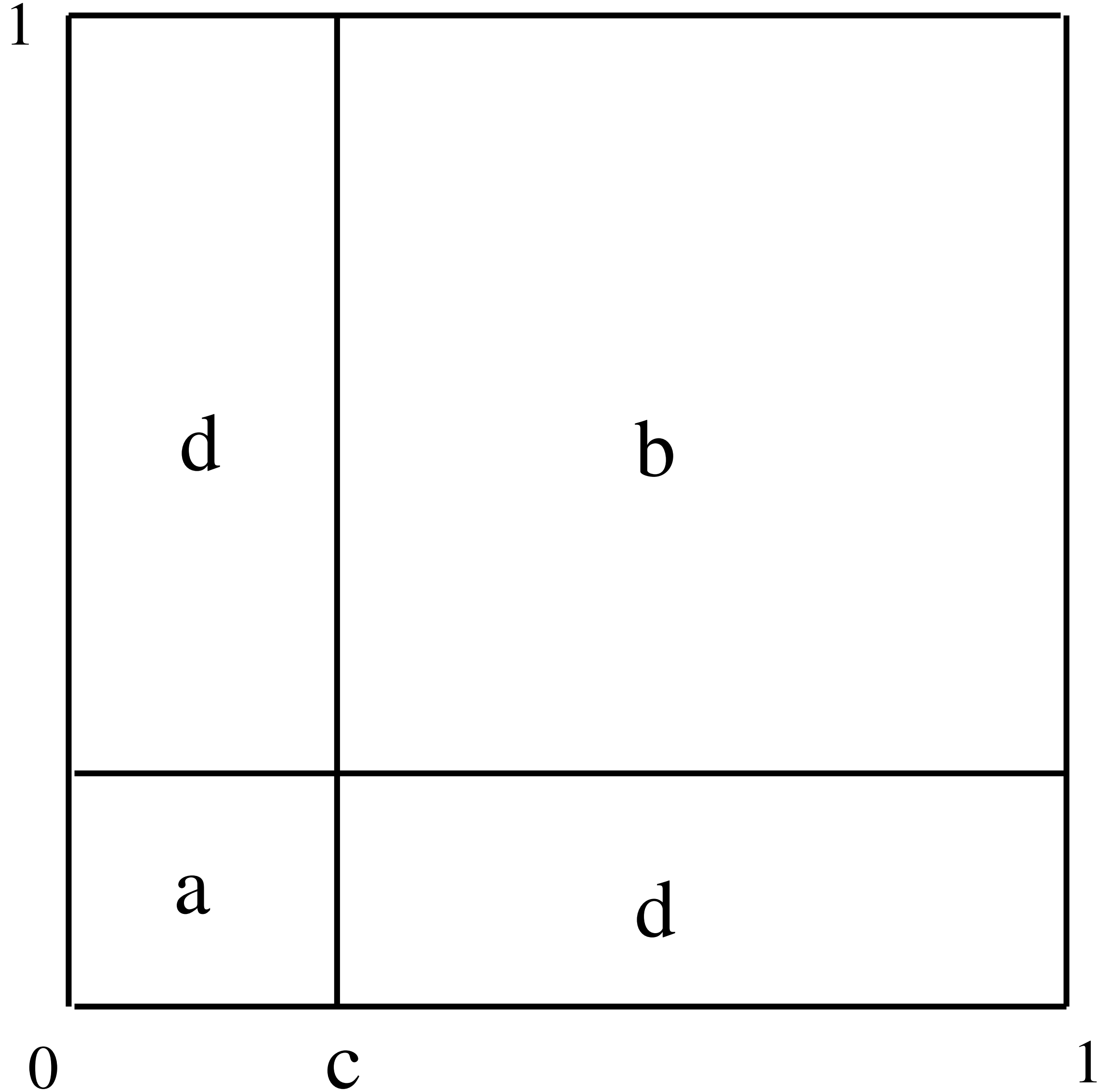
$$-\int_{[0,1]^2} \frac{1}{2}\{q(x,y)\ln[q(x,y)] + [1-q(x,y)]\ln[1-q(x,y)]\}\,dxdy$$

and the densities $t_\varepsilon(q)$ and $t_\tau(q)$ are given by:

$$t_\varepsilon(q) = \int_{[0,1]^2} q(x,y)\,dxdy; \;\; t_\tau(q) = \int_{[0,1]^3} q(x,y)q(y,z)q(z,x)\,dxdy.$$

Our recent results: For each of two open sets in the parameter plane, separated by the ER curve, we determine unique $S(q)$-optimal graphons $q_{\varepsilon,\tau}$ at each point (ε,τ); the $q_{\varepsilon,\tau}$ are bipodal with 4 real parameters which are real analytic in ε and τ and can be determined to arbitrary accuracy.





The parameters of a bipodal graphon

Using this drop in degrees of freedom we prove that these define a pair of 2 dimensional analytic surfaces in 4 dimensions, with a common boundary of singularities.

More specifically, in terms of the function

$$H(p) = -[p\ln(p) + (1-p)\ln(1-p)]$$

of the real variable p we have proven:

Theorem 1. There is an open subset $\mathcal{O}_1$ in the planar set of achievable parameters (ε, τ), whose upper boundary is the curve $\tau = \varepsilon^3$, $1/2 < \varepsilon < 1$, such that at (ε, τ) in $\mathcal{O}_1$ there is a unique entropy-optimizing graphon $g_{(\varepsilon,\tau)}$. This graphon is bipodal and for fixed $(\varepsilon, \tau) = (e, e^3 - \delta^3)$, the values of a, b, c, d can be approximated to arbitrary accuracy via an explicit iterative scheme. These parameters can also be expressed via asymptotic power series in δ whose leading terms are:

$$
\begin{aligned}
a &= 1 - e - \delta + O(\delta^2) \\
b &= e - \frac{\delta^2}{2e - 1} + O(\delta^3) \\
c &= \frac{\delta}{2e - 1} - \frac{2\delta^2}{2e - 1} + O(\delta^3) \\
d &= e + \delta + \frac{\delta^2}{eH'(e)} \left(H'(e) - \left(e - \frac{1}{2}\right) H''(e) \right) + O(\delta^3).
\end{aligned}
$$

Theorem 2. There is an open subset $\mathcal{O}_2$ in the planar set of achievable parameters (ε, τ), whose lower boundary is the curve $\tau = \varepsilon^3$, $1/2 < \varepsilon < 1$, such that at each (ε, τ) in $\mathcal{O}_2$ there is a unique entropy-optimizing graphon $g_{(\varepsilon,\tau)}$. This graphon is bipodal and for fixed $(\varepsilon, \tau) = (e, e^3 + \Delta\tau)$ the values of a, b, c, d can be approximated to arbitrary accuracy via an explicit iterative scheme. These parameters can also be expressed via asymptotic power series in $\Delta\tau$ whose leading terms are:

$$
\begin{aligned}
a &= a_0 + O(\Delta\tau) \\
b &= e - \frac{2\Delta\tau}{3e(2e-1)} + O([\Delta\tau]^2) \\
c &= \frac{\Delta\tau}{3e(2e-1)^2} + O([\Delta\tau]^2) \\
d &= 1 - e + O(\Delta\tau),
\end{aligned}
$$

where a_0 is the solution to

$$H'(a_0) = \left(1 - \frac{2}{e}\right) H'(e).$$

Connection with finite graphs. If graphon q optimizing $S(q)$ is unique under given constraints (ε, τ), then as the number of nodes n diverges and the window $\delta_n \to 0$, exponentially most graphs G with densities $\varepsilon(G) \in (\varepsilon - \delta_n, \varepsilon + \delta_n)$ and $\tau(G) \in (\tau - \delta_n, \tau + \delta_n)$ will have reduced $0 - 1$ graphon close to q in cut metric.

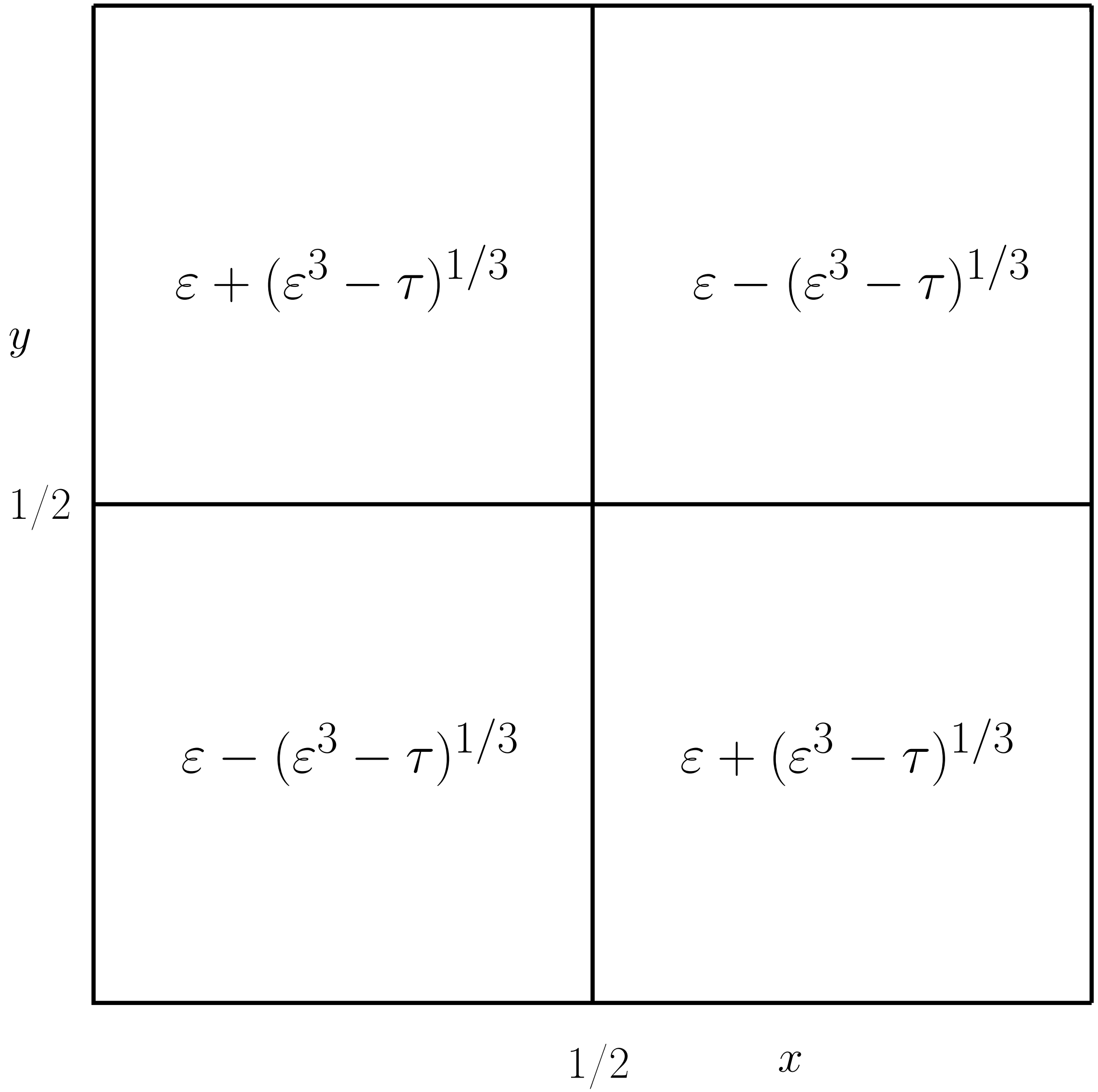
Summary: In conflicting-constraints for graphs we know more than for sphere packing and permutations; we know *quantitatively*, to any desired accuracy, how the system adjusts to the conflict, mostly smoothly but with occasional singularity.

Open problems:

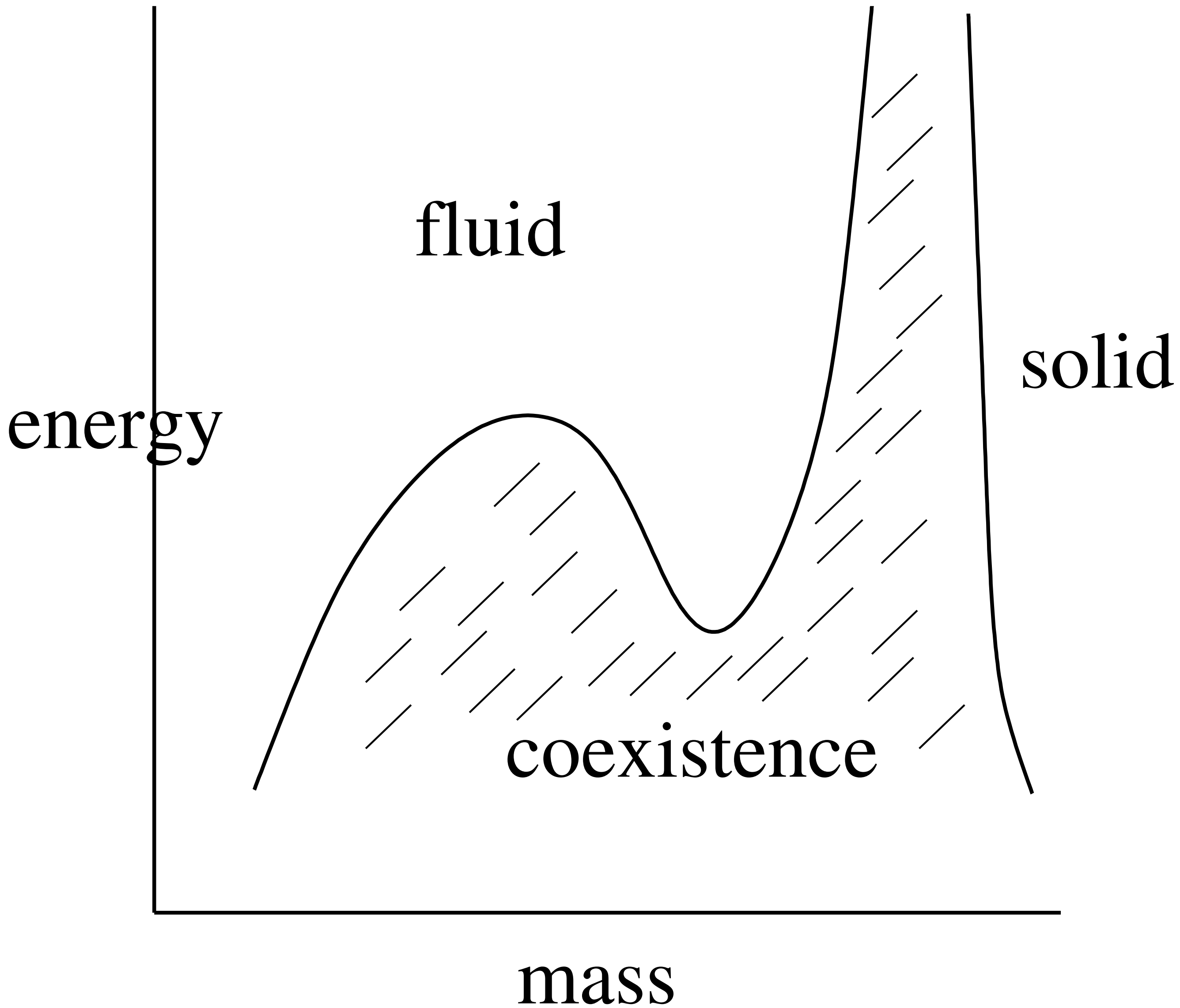
symmetry as an order parameter near edge density 1/2

discontinuous transition

behavior near $(\varepsilon, \tau) = (1/2, 1/8)$



Symmetric graphon, proven extremal for $\varepsilon = 1/2, \;\; 0 \leq \tau \leq 1/8$


fluid
solid
energy
coexistence
mass

It was Landau (1958) who, long ago, first pointed out the vital importance of symmetry in phase transitions. This, the First Theorem of solid-state physics, can be stated very simply: it is impossible to change symmetry gradually. A given symmetry element is either there or it is not; there is no way for it to grow imperceptibly. This means, for instance, that there can be no critical point for the melting curve as there is for the boiling point: it will never be possible to go continuously through some high-pressure phase from liquid to solid.

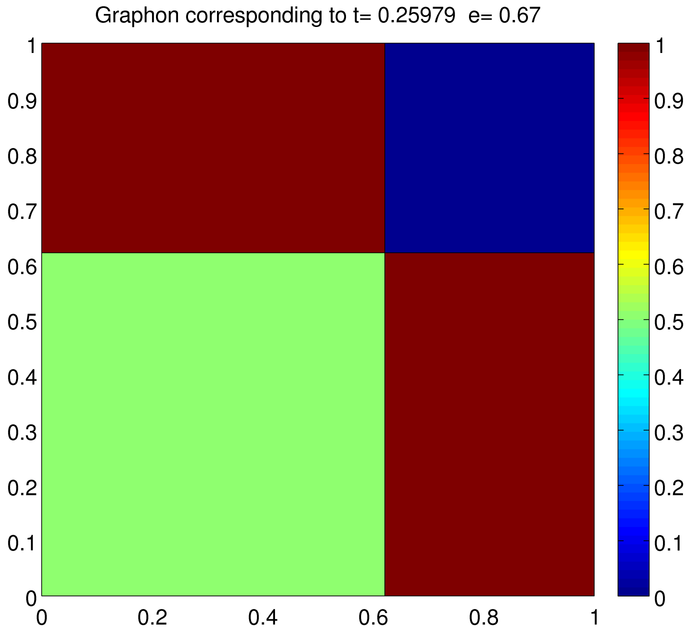
P.W. Anderson, Basic Notions of Condensed Matter Physics, (1984), p. 19

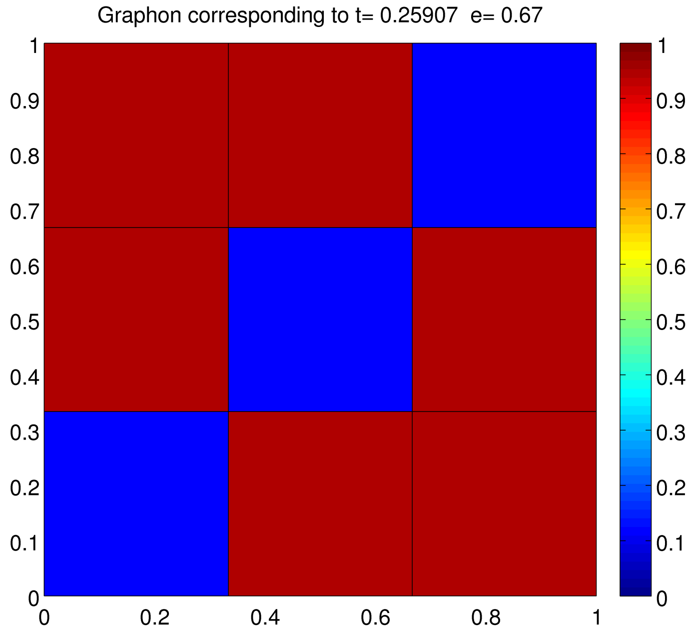
This is the theoretical argument, which has appeared to some to be a little too straightforward to be absolutely convincing.

A.B. Pippard, Classical Thermodynamics (1957), p. 122

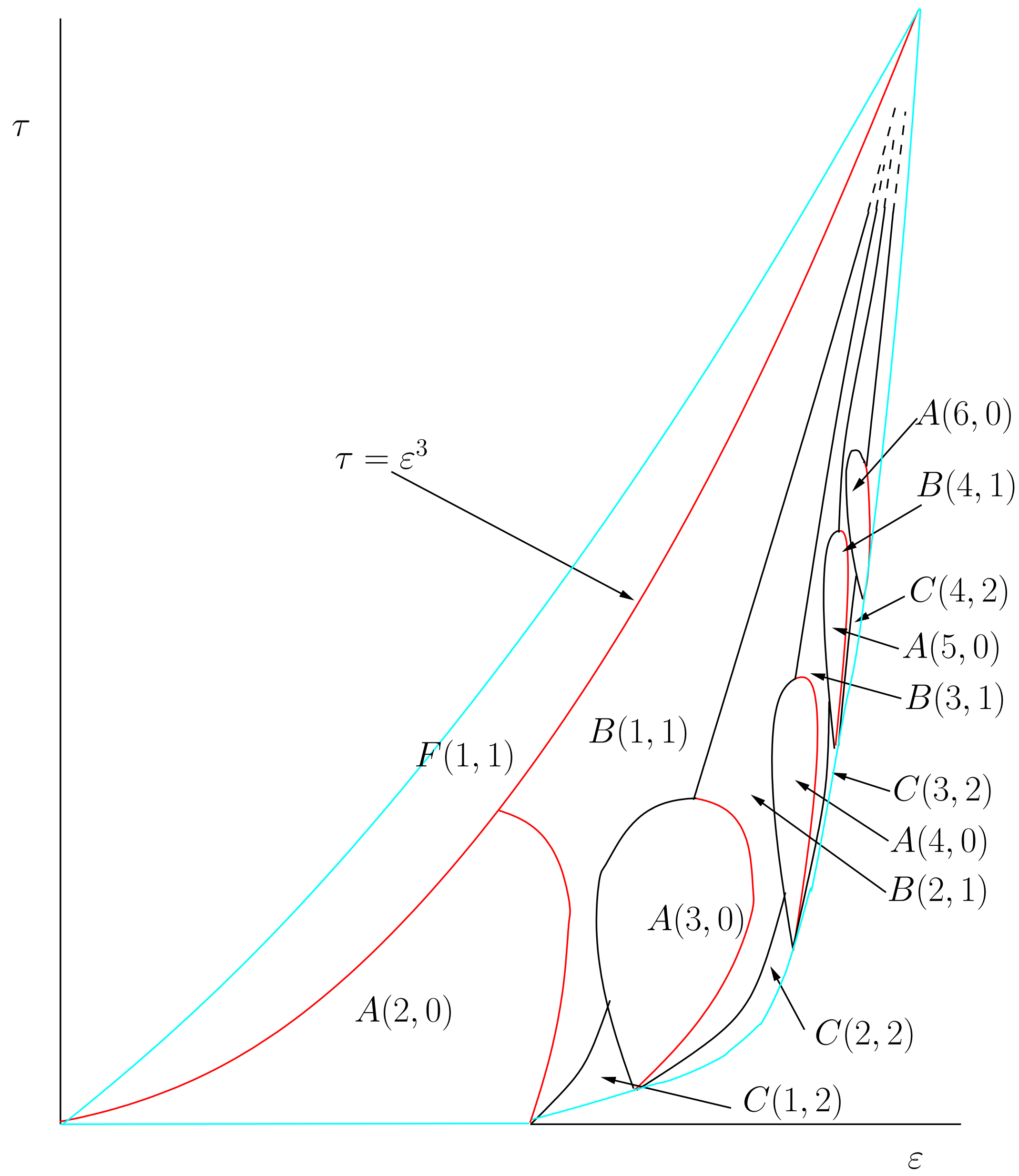
Problem: Show that $(c - 1/2)^2 = 0$ in an open set near $\varepsilon = 1/2$.

In summary, if one can construct an ‘order parameter’ associated with the optimal graphons $q_{\varepsilon,\tau}$, which is real *analytic* in ε and τ, positive in one parameter region and (constant) zero in another region, one has a powerful method for understanding why the system cannot be connected smoothly between such parameter regions.





Transition between phases $B(1,1)$ and $A(3,0)$ at edge density 0.670
Triangle densities: 0.25979, 0.25907



τ
$\tau = \varepsilon^3$
$A(6,0)$
$B(4,1)$
$C(4,2)$
$A(5,0)$
$B(3,1)$
$B(1,1)$
$F(1,1)$
$C(3,2)$
$A(4,0)$
$B(2,1)$
$A(3,0)$
$A(2,0)$
$C(2,2)$
$C(1,2)$
ε